

Nonane

111-84-2 | DTXSID9025796

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 146 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 9.30e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nonane</div> <div>Measured: 151</div> <div>Predicted: 146</div>	<div>Image not found</div> <div>Heptane, 4-ethyl-</div> <div>Measured: 141</div> <div>Predicted: 143</div>	<div>Image not found</div> <div>3-Methyloctane</div> <div>Measured: 144</div> <div>Predicted: 143</div>
<div>Image not found</div> <div>4-Methyloctane</div> <div>Measured: 142</div> <div>Predicted: 143</div>	<div>Image not found</div> <div>2-Methyloctane</div> <div>Measured: 143</div> <div>Predicted: 143</div>	